Multicomponent WKB on arbitrary symplectic manifolds: A star product approach

C. Emmrich, H. Römer
Fakultät für Physik
Universität Freiburg
Hermann-Herder-Straße 3
79104 Freiburg

Abstract

It is known that in the WKB approximation of multicomponent systems like Dirac equation or Born-Oppenheimer approximation, an additional phase appears apart from the Berry phase. So far, this phase was only examined in special cases, or under certain restrictive assumptions, namely that the eigenspaces of the matrix or endomorphism valued symbol of the Hamiltonian form trivial bundles.

We give a completely global derivation of this phase which does not depend on any choice of local trivializing sections. This is achieved using a star product approach to quantization. Furthermore, we give a systematic and global approach to a reduction of the problem to a problem defined completely on the different "polarizations". Finally, we discuss to what extent it is actually possible to reduce the problem to a really scalar one, and make some comments on obstructions to the existence of global quasiclassical states.

1 Introduction

Whereas the semiclassical and WKB approximation of systems with Hamiltonians whose symbol is a scalar function is very well understood both on a local and a global level, this is not the case to the same extent for systems with Hamiltonians whose symbol are matrix valued functions on a symplectic manifold, or sections in the endomorphism bundle of a vector bundle over a symplectic manifold M.

Such Hamiltonians appear in many places in physics: Examples are the Dirac equation, multicomponent wave equations like electrodynamics in media and Yang-Mills theories, and the Born-Oppenheimer approximation in molecular physics.

In the scalar case, a nice geometric interpretation of the semiclassical states as half densities on Lagrangian submanifolds invariant under the Hamiltonian flow exists, and discrete spectra may be computed using the Bohr-Sommerfeld condition, taking into account the Maslov correction.

In the multicomponent case, the analogous structures are not known: There exist many results on a local level, but on a global level results are only known either for special examples, or under the very restrictive assumption that the eigenspaces of the symbol of the Hamiltonian form trivial bundles over the symplectic base manifold M [16, 14, 15].

Locally, the WKB ansatz for multicomponent systems still is

$$\Psi(x) = a(x,\hbar)\exp(iS(x)/\hbar)$$

with $a(x,\hbar) = a_0(x) + a_1(x)\hbar + ...$ Here, the $a_i(x)$ are now vector valued functions [10, 13, 16].

In lowest order in $\hbar$ the time independent Schrödinger equations yields:

$$\big[H_0\big(x, dS(x)\big) - E\big]a_0(x) = 0,$$

i.e., $a_0(x)$ has to be an eigenvector of the matrix valued principal symbol $H_0(x,p)$ at the point $p = dS(x)$. Denoting by $\lambda_\alpha(x,p)$ the α-th eigenvalue of the matrix $H_0(x,p)$ at the point (x,p), the phase $S(x)$ has to satisfy the Hamilton-Jacobi-equation for one of the eigenvalue functions λ_α: $\lambda_\alpha(x, dS) - E = 0$, and one obtains a separate phase function for each "polarization" α.

The equation of order $\hbar$ has a more complicated structure than in the scalar case: The absolute value of the amplitude still fulfills the usual transport equation, but the vector a_0 satisfies a more complicated equation which contains a Berry phase term, and an additional term without obvious geometric meaning [18, 15, 13].

There exist some functional analytically rigorous results on the WKB approximation for special systems in the literature [16, 14]. However, no analog of the Bohr-Sommerfeld quantization condition is known in general, and all those results have the common feature that they are based on the assumption that the bundles of eigenvectors of the symbol of the Hamiltonian are trivial, at least on the "classically allowed region" $\lambda_\alpha < \tilde{E}$ for an $\tilde{E} > E$. This assumption is not fulfilled in many physical applications: Apart from cases like the Dirac equation on topologically non-trivial space-times, where the possibility of non-trivial eigenbundles is quite obvious, this phenomenon even arises in applications to the Born-Oppenheimer approximation: Although the nuclear phase space is contractible, non-trivial bundles may arise due to the phenomenon of level crossing, i.e., the possibility of two eigenvalues becoming equal in certain points on phase space: The degeneracy increases in those points. For the WKB approximation one has to cut out those points and to treat them separately. This may lead to the appearance of non-trivial bundles, and as a matter of fact, it is well known that non-trivial bundles play a role in real molecular systems.

In [15] a Bohr-Sommerfeld condition could be derived for systems whose symbol has non-degenerate eigenvalues, using the Moyal product on matrix valued symbols in order to reduce this case to the WKB approximation for a scalar system. To this end, a formally unitary $U = U_0 + U_1\hbar + ...$ was introduced such that

$$U^\dagger * H * U = \Lambda$$

for some diagonal matrix valued symbol Λ.

However, this method has several disadvantages: First, considering this equation at zeroth order, one concludes that the columns of U_0 are eigenvectors of H_0. Hence, this method may again be applied globally only if the eigenvector bundles are trivial. Moreover, it is not possible to generalize this method to the case of degenerate eigenvalues with constant degeneracies. In this case, it is in general not possible to diagonalize the Hamiltonian globally (even if the eigenvector bundles are trivial), but only to block-diagonalize it. Finally, this approach is not natural from a geometric point of view: The Moyal product is defined only on trivial bundles over $\mathbb{R}^{2n}$, hence it is not possible to stick with the Moyal product if one wants to reduce the problem in a global way to a problem defined on the respective eigenbundles. In particular, it will become obvious that this method, if generalized to the degenerate case, will correspond to a quantization based on a non-canonical and unnatural choice of a connection: The choice of U_0 implies, as mentioned above, a choice of trivializing sections of the eigenbundles. In a sense to become clear in section 4, the quantization achieved by this process corresponds to a connection with respect to which the chosen set of trivializing sections is covariantly constant. Such a connection is obviously geometrically meaningless, since it depends on the choice of those sections.

The goal of this article is to reduce the problem of WKB for endomorphism valued symbols "as far as possible" to the scalar case, using only globally defined methods: Apart from being an important progress in a geometric understanding of multicomponent WKB approximation, this is an important step towards a Bohr-Sommerfeld like condition, since the latter is necessarily global in nature.

For this reduction of the problem, the notion of star products on arbitrary endomorphism bundles proves to be particularly useful, since we have to deal with non-trivial bundles. Such star products are known to exist on arbitrary endomorphism bundles over a symplectic manifold, as has been shown by Fedosov [8]. His method is particularly adapted to our purposes, since his proof of existence is constructive in nature, and there exist explicit formulas for the isomorphisms of different star products. Although we will restrict ourselves to formal star products, i.e., to formal power series in $\hbar$, the method can in principle be translated into operator language using the notion of asymptotic operator representations, which are, in a suitable sense, representations up to order $O(\hbar^\infty)$ of the star product algebra. Such representations are known to exist if certain quantization condition are satisfied [9].

The main idea of the paper is to give a "basis independent and geometrically natural version of the diagonalization procedure of [15]". What is meant by this becomes more apparent if one observes that essentially all additional complications in the WKB approximation of multicomponent systems are due to the fact that the projection operators onto the eigenspaces of the principal symbol of H are in general not constant. If one could replace ordinary derivatives by covariant derivatives with respect to which the projections are covariantly constant, the problem would be considerably simplified. However, as we assume that we are studying a given definite quantum mechanical system, we cannot simply replace ordinary derivatives by covariant derivatives "by hand", as we do not want to change the physics of the

system.

Here, the use of Fedosov's star product proves to be particularly powerful: His construction of a star product depends on the choice of a symplectic connection on the base space and a connection on the endomorphism bundle. Nevertheless, the different star products are isomorphic. Hence, if we interpret the choice of the connection as defining a definite quantization procedure, then we may change this connection without changing physics if we apply at the same time the corresponding isomorphism. This means that we are allowed to change the connection in order to simplify the problem, if we consistently correct the symbols of the Hamiltonian and all interesting observables at the same time.

Indeed, this additional freedom (which is completely missing if one restricts oneself to the Moyal product) may be used to simplify the problem considerably: One may find an $\hbar$-dependent connection, $\hbar$-dependent projections, and a corrected symbol such that all these structures are compatible in an obvious sense. An important feature of Fedosov's product is that the star product constructed from these data is compatible with the projections as well, i.e,. if A and B are observables such that there corrected symbols commute with the projections, then the corresponding star product $A * B$ commutes with the projections as well. Hence, the different blocks defined by the projections are decoupled for a suitable set of observables.

Using these techniques, we will be lead to a geometrical interpretation of the additional phases appearing in the WKB approximation at order $\hbar$ as formed from the Poisson-curvature and an analog of the second fundamental form of a Berry-type connection. We will show that this even holds if one chooses a different connection for computing the correction. Hence, the Berry type connection is distinguished among the set of all compatible connections.

The paper is organized as follows: In the next section we give a short overview over Fedosov's construction of star products on arbitrary endomorphism bundles to the extent needed for our applications. The main fact will be that a modification of the connection on the endomorphism bundle at some order $O(\hbar^k)$ induces an isomorphism of the corresponding star product algebras which implies corrections only at higher order $O(\hbar^{k+1})$. This will allow the use of inductive methods in the main part of the paper, and to compute the corrections iteratively order by order in $\hbar$.

In section 3, we show how one may use the freedom of choosing the connection in order to block-diagonalize the system, i.e., to find a decomposition of the vector bundle such that the Hamiltonian and a large class of observables preserve this decomposition at the quantum mechanical level. Furthermore, we will show that for a suitable class of observables, a formal Heisenberg equation of motion may be defined.

In section 4 we compute the correction of the symbol of H at order $\hbar$ for all compatible connections, thus reproducing in particular the additional phase observed in special cases before. We give a geometric interpretation of these terms, and show that a certain adapted connection which is of "Berry type" is distinguished among all adapted connections.

Finally, in section 5 we examine to which extent it is actually possible to reduce the problem to a scalar one, and discuss some aspects connected to a Bohr-Sommerfeld like quantization condition.

2 Star products on endomorphism bundles

In this section we give a short introduction to Fedosovs approach to deformation quantization [8], as needed for our purposes, and we prove three lemmas needed in section 3

We assume the reader to be familiar with the general ideas of deformation quantization. For an introduction, we refer to [2].

We denote the Moyal product, which is the star product on $\mathbb{R}^{2n}$ corresponding to Weyl ordering, by $\diamond$:

$$(a \diamond b)(x) = (e^{\frac{i\hbar}{2}\omega^{kl}\frac{\partial}{\partial x^k}\frac{\partial}{\partial y^l}} a(x)b(y))\Big|_{x=y},$$

where ω^{kl} are the components of the Poisson tensor. The algebra $\mathcal{F}(\mathbb{R}^{2n}) \otimes \mathbb{C}[[\hbar]]$ with the product $\diamond$ is called the *Weyl algebra* over $\mathbb{R}^{2n}$. (Here, $\mathcal{F}(\mathbb{R}^{2n})$ denotes the algebra of smooth functions on $\mathbb{R}^{2n}$.)

Let M be a symplectic manifold with symplectic form ω and a symplectic connection ∂_s (such a connection always exists), and let V be a hermitian vector bundle over M with hermitian connection ∇. We consider the bundle $V[[\hbar]] = V \otimes \mathbb{C}[[\hbar]]$ which is a fiber bundle over M whose fiber over a point $q \in M$ is the $\mathbb{C}[[\hbar]]$ module $V_q[[\hbar]] = V_q \otimes \mathbb{C}[[\hbar]]$. Let $E[[\hbar]] = \bigcup_{q\in M} End(V_q) \otimes \mathbb{C}[[\hbar]]$ be the bundle of endomorphism s of the fibers of $V[[\hbar]]$.

We may define a star product on the endomorphims $\Gamma(E[[\hbar]])$ of the bundle $V[[\hbar]]$ by Fedosov's construction [8]. To this end one considers the algebra

$$\mathcal{A} = \Gamma(E[[\hbar]] \otimes W),$$

where W is the Weyl algebra bundle over M (i.e., the bundle over M whose fiber over q consists of Weyl algebra on the symplectic vector space T_qM).

$\mathcal{A}$ is graded as a vector space, with a degree defined by:

$$deg(\hbar) = 2, \quad deg(y^i) = 1,$$

where the (y^i) are coordinates on the fiber T_qM. Defining $\mathcal{A}_i$ as the set of all $\hat{X} \in \mathcal{A}$ which are sums of terms of degree larger or equal i, $\mathcal{A}$ becomes a filtered algebra:

$$\mathcal{A} = \mathcal{A}_0 \supset \mathcal{A}_1 \supset \ldots.$$

The hermitian connection ∇ on V induces a connection on $E[[\hbar]]$ which we denote by ∇ as well. Together with the symplectic connection ∂_s on M this defines a connection $\partial = 1 \otimes \partial_s + \nabla \otimes 1$ on $E[[\hbar]] \otimes W$.

One may construct by an iterative procedure, starting with ∂, an exterior covariant derivative D on $\mathcal{A} \otimes \Omega(M)$, the forms on M with values in $\mathcal{A}$, such that

1. $D^2 = 0$
2. the space of covariant constant elements in $\mathcal{A}\hat{=}\mathcal{A}\otimes\Omega_0(M) \subset \mathcal{A}\otimes\Omega(M)$ is isomorphic as a vector space to $E[[\hbar]]$
3. D acts as a derivation on $\mathcal{A}\otimes\Omega(M)$ (with the product induced by the Moyal product on $\mathcal{A}$).

These properties guarantee that the covariant constant sections form a subalgebra and allow us to use the vector space isomorphism of 2. between the covariant constant elements in $\mathcal{A}$ and $E[[\hbar]]$ to define the star product on $\Gamma(E[[\hbar]])$ by pull back of the product on $\mathcal{A}$. More precisely, if we denote the isomorphism from $\Gamma(E[[\hbar]])$ to the covariantly constant elements in $\mathcal{A}$ by $\mathcal{Q}$, and its inverse by σ, the star product on $E[[\hbar]]$ is given by:

$$a * b = \sigma(\mathcal{Q}(a) \diamond \mathcal{Q}(b))$$

for $a, b \in \Gamma(E[[\hbar]])$.

To give an explicit expression for this flat derivative, we introduce operators δ and δ^{-1} on $\mathcal{A}\otimes\Omega(M)$:

$$\delta = dx^i \wedge \frac{\partial}{\partial y^i}$$

and

$$\delta^{-1}a = \frac{1}{p+q} i_{y^i \frac{\partial}{\partial x^i}} a$$

if a is a q-form that is homogeneous of degree p in the fiber coordinate y, $p+q \neq 0$, and $\delta^{-1}a = 0$ if $p = q = 0$. These operators have the important property that for any $\hat{X} \in \Omega(M)\otimes\mathcal{A}$:

$$\hat{X} = \hat{X}_{00} + (\delta^{-1}\delta + \delta\delta^{-1})\hat{X}$$

Here, $\hat{X}_{00}$ denotes the part of $\hat{X}$ that is a zero form of degree 0 in y.

The ansatz

$$D = -\delta + \partial + \left[\frac{i}{\hbar} r, \ \right]$$

for a one form r with values in $\mathcal{A}$, the flatness condition $D^2 = 0$ together with a "normalization condition" $\delta^{-1}r = 0$ leads to the condition

$$r = \delta^{-1}\tilde{R} + \delta^{-1}\left(\partial r + \frac{i}{\hbar} r^2\right), \tag{1}$$

by which r is uniquely defined and may be computed iteratively. Here, $\tilde{R}$ is the curvature of the connection ∂, considered as a two form with values in $\mathcal{A}$, acting on $\mathcal{A}$ as $\frac{i}{\hbar}[\tilde{R}, \cdot]$: If R^E is the curvature of ∇ and R^s is the curvature of ∂_s, then $\tilde{R}$ is locally given by:

$$\tilde{R} = -i\frac{\hbar}{2} R^E_{ij} dx^i \wedge dx^j + 1 \otimes \frac{1}{4}\omega_{ij}(R^s)^i_{klm} y^j y^k dx^l \wedge dx^m.$$

We note that in spite of the factor $1/\hbar$ in (1) the solution of this equation is a power series in $\hbar$, containing no negative powers.

With r determined, the covariantly constant continuation $\mathcal{Q}(a)$ of a in $\mathcal{A}$ is given by the unique solution to the equation

$$\mathcal{Q}(a) = a_0 + \delta^{-1}(\partial\mathcal{Q}(a) + [\frac{i}{\hbar}r, \mathcal{Q}(a)]), \tag{2}$$

which may again be solved iteratively.

Different choices of ∇ will yield different star products. However, they are equivalent in the following sense:
Given two hermitian connections $\nabla^{(1)}, \nabla^{(2)}$ and two symplectic connections $\partial_s^{(1)}, \partial_s^{(2)}$ with corresponding derivates $D^{(1)}, D^{(2)}$, there is a formally unitary

$$U_{(12)} = \exp_\diamond(\frac{i}{\hbar}A_{(12)})$$

for some $A \in \mathcal{A}$ such that:

$$D^{(1)}\hat{X} = 0 \Rightarrow D^{(2)}(U_{(12)} \diamond \hat{X} \diamond U_{(12)}^{-1}) = 0$$

for any $\hat{X} \in \Gamma(\mathcal{A})$. (Here, $\exp_\diamond$ denotes the exponential with respect to the fibrewise Moyal product $\diamond$.)

Furthermore, letting $\mathcal{Q}^{(i)}(X)$ denote the covariant constant continuation of $X \in \Gamma(E[[\hbar]])$ with respect to $D^{(i)}$, and $\sigma^{(i)}$ denote the inverse of $\mathcal{Q}^{(i)}$ $(i = 1, 2)$, we have an isomorphism of the different star-products given by:

$$\phi(X) \stackrel{\text{def}}{=} \sigma^{(2)}(U_{(12)} \diamond \mathcal{Q}^{(1)}(X) \diamond U_{(12)}^{-1})$$

To check this statement one simply has to compute:

$$\begin{aligned}
\phi(X *_1 Y) &= \sigma^{(2)}(U_{(12)} \diamond \mathcal{Q}^{(1)}(X *_1 Y) \diamond U_{(12)}^{-1}) \\
&= \sigma^{(2)}(U_{(12)} \diamond \mathcal{Q}^{(1)}(X) \diamond \mathcal{Q}^{(1)}(Y) \diamond U_{(12)}^{-1}) \\
&= \sigma^{(2)}((U_{(12)} \diamond \mathcal{Q}^{(1)}(X) \diamond U_{(12)}^{-1}) \diamond (U_{(12)} \diamond \mathcal{Q}^{(1)}(Y) \diamond U_{(12)}^{-1})) \\
&= \sigma^{(2)}(\mathcal{Q}^{(2)}(\phi(X)) \diamond \mathcal{Q}^{(2)}(\phi(Y)) \\
&= \phi(X) *_2 \phi(Y)
\end{aligned}$$

We note that, in general, $\phi(X) \neq X$. This is precisely what was meant in the introduction by the statement that we can change the quantization procedure without changing physics, if we consistently correct the symbols of the Hamiltonian and the relevant observables at the same time.

We may express $U_{(12)} \diamond \hat{X} \diamond U_{(12)}^{-1}$ directly in terms of $A_{(12)}$ as:

$$U_{(12)} \diamond \hat{X} \diamond U_{(12)}^{-1} = \sum_{k=0}^{\infty} \left(\frac{i}{\hbar}\right)^k \frac{1}{k!} \underbrace{[A_{(12)}, [A_{(12)}, \ldots [A_{(12)}}_{\text{k-times}}, \hat{X}] \ldots]] \tag{3}$$

For $A_{(12)}$, one may derive the following equation which defines it iteratively [8]:

$$A_{(12)} = \delta^{-1}\left(\frac{ad(\frac{i}{\hbar}A_{(12)})}{\exp_\diamond(ad(\frac{i}{\hbar}A_{(12)}))-1}(\Delta\gamma)_{(12)} + (D+\delta)A_{(12)}\right) \tag{4}$$

Here, $(\Delta\gamma)_{(12)}$ denotes the one form on M with values in $\mathcal{A}$ (acting by $\frac{i}{\hbar}[(\Delta\gamma)_{(12)},\cdot]$) which is induced by the difference of the two connection forms corresponding to $\partial^{(i)} = 1\otimes\partial_s^{(i)} + \nabla^{(i)}\otimes 1,\ i=1,2$ on $E[[\hbar]]\otimes W$. (The difference of two connection forms is tensorial and hence defines a one form on M). If $\nabla^{(i)}$ is locally given by $\frac{\partial}{\partial x^i}+\Gamma_i$, and the Christoffel symbols corresponding to $\partial_s^{(i)}$ are given by $(\Gamma_s^{(i)})^k_{lm}$, then $(\Delta\gamma)_{(12)}$ is locally given by

$$(\Delta\gamma)_{12} = -i\hbar(\Gamma_i^{(2)}-\Gamma_i^{(1)})dx^i + 1\otimes\frac{1}{2}\omega_{ij}\left((\Gamma_s^{(2)})^i_{kl}-(\Gamma_s^{(1)})^i_{kl}\right)y^jy^kdx^l \tag{5}$$

In particular, it is obvious from this expression that $A_{(12)}$ does not contain any negative powers of $\hbar$.

Remarks:

1.) Though U does contain inverse powers of $\hbar$, $U_{(12)}\diamond\hat{X}\diamond U_{(12)}^{-1}$ is again a power series in $\hbar$ for all $\hat{X}\in\Gamma(\mathcal{A})$ with $D^{(1)}\hat{X}=0$. This is shown in [8] by showing first that $D^{(2)}(U_{(12)}\diamond\hat{X}\diamond U_{(12)}^{-1})=0$ in an enlarged algebra W^+ whose elements may contain negative powers of $\hbar$ in some specified way, and then showing that any $Y\in W^+$ such that $D^{(2)}Y=0$ and such that $\sigma^{(2)}(Y)$ is a power series in $\hbar$, lies in the subalgebra W itself.

2.) The mappings $\sigma^{(i)}$ may be considered as the restriction of one mapping σ from $\mathcal{A}$ to $\Gamma(E[[\hbar]])$. This mapping is simply given by setting y to zero, i.e., it picks out the part of $\hat{X}\in\mathcal{A}$ not depending on y. We will use the notions of [8] and call $\sigma(\hat{X})$ the *symbol* of $\hat{X}\in\mathcal{A}$.

From now on we will restrict ourselves to one fixed symplectic connection ∂_s on M and will only modify the connection ∇ on V. We will prove two lemmas which will be essential in the following sections.

Lemma 1 *Let $\nabla^{(1)}$ and $\nabla^{(2)}$ be connections on $E[[\hbar]]$, ∂_s a fixed symplectic connection, and let $D^{(1)},D^{(2)}$ denote the corresponding flat Fedosov connections, and $U_{(12)}$ the corresponding automorphism. Assume that the difference of the two connections $\nabla^{(1)}$ and $\nabla^{(2)}$ is of order $O(\hbar^m)$ for some m. Then:*

$$\sigma(U_{(12)}\diamond\hat{X}\diamond U_{(12)}^{-1}) = \sigma(\hat{X}) + O(\hbar^{(m+1)})$$

for any $\hat{X}\in\mathcal{A}$ which is covariantly constant with respect to $D^{(1)}$.

Proof: By (5), $A_{(12)}$ is contained in $\mathcal{A}_{2m+3}$. Hence, using (3), we may conclude that $U_{(12)}\diamond\hat{X}\diamond U_{(12)}^{-1}-\hat{X}\in\mathcal{A}_{2m+1}$, and the symbols $\sigma(U_{(12)}\diamond\hat{X}\diamond U_{(12)}^{-1}),\sigma(\hat{X})$ may differ only by a term of order $O(\hbar^{m+1})$. Q.E.D.

If we consider three different connections, $U_{(13)}$ is not necessarily the same as the composition $U_{(23)} \diamond U_{(12)}$ of $U_{(12)}$ and $U_{(23)}$, but $U_{(13)}^{-1} \diamond U_{(23)} \diamond U_{(12)}$ defines an automorphism of the elements in $\mathcal{A}$ covariantly constant with respect to $D^{(1)}$. Although this automorphism in general is not simply the identity, we have the following lemma:

Lemma 2 *Let $\nabla^{(1)}$, $\nabla^{(2)}$, and $\nabla^{(3)}$ be connections on $E[[\hbar]]$, ∂_s a fixed symplectic connection, and let $D^{(i)}$ denote the corresponding flat Fedosov connections and $U_{(ik)}$ the corresponding automorphisms of $\mathcal{A}$ mapping covariant constant sections with respect to $D^{(i)}$ to covariant constant sections with respect to $D^{(k)}$. Assume that the difference of the two connections $\nabla^{(2)}$ and $\nabla^{(3)}$ is of order $O(\hbar^m)$ for some m. Then:*

$$\sigma(U_{(13)} \diamond \hat{X} \diamond U_{(13)}^{-1}) = \sigma((U_{(23)} \diamond U_{(12)}) \diamond \hat{X} \diamond (U_{(23)} \diamond U_{(12)})^{-1}) + O(\hbar^{(m+2)})$$

for any $\hat{X} \in \mathcal{A}$ which is covariantly constant with respect to $D^{(1)}$

Proof: By the Baker-Campbell-Hausdorff formula, $U_{(23)} \diamond U_{(12)}$ may be written as $\exp_\diamond(\frac{i}{\hbar}A)$ with $A = A_{(12)} + A_{(23)} + C$, where C is the sum of multiple commutators of $\frac{1}{\hbar}A_{(12)}$ and $\frac{1}{\hbar}A_{(23)}$ multiplied by $\hbar$. From formulas (4) and (5) it is obvious that A does not contain negative powers of $\hbar$.

Now, by assumption and (4), (5), $A_{(23)}$ is contained in $\mathcal{A}_{2m+3}$, and is of the special form:

$$A_{23} = \hbar^{m+1}T^1_{(23)} + \hbar^m T^2_{(23)} + T^3_{(23)}$$

where $T^1_{(23)}$ contains only terms at least of degree 1 in the fiber coordinate y, $T^2_{(23)}$ contains only terms at least of degree 3 in y, and $T^3_{(23)} \in \mathcal{A}_{2m+4}$.

Similarly, $A_{12} = \hbar T^1_{12} + T^2_{12} + T^3_{12}$ with $T^1_{(12)}$ containing only terms at least of degree 1 in the fiber coordinate y, $T^2_{(12)}$ containing only terms at least of degree 3 in y, and $T^3_{(12)} \in \mathcal{A}_4$. Now, since all other terms in the Baker-Cambell-Hausdorff formula will be contained in $\mathcal{A}_{2m+5}$, we may conclude that

$$C = \frac{1}{\hbar}[\hbar T^1_{12} + T^2_{12}, \hbar^{m+1}T^1_{12} + \hbar^m T^2_{12}] + ...,$$

where the missing terms denoted by dots are in $\mathcal{A}_{2m+5}$. An inspection of each term, using the fact that T^2_{12}, T^2_{23} are scalar, finally shows that C is of the form:

$$C = \hbar^m C^1 + \hbar^{m+1}C^2 + \hbar^{m+2}C^3 + C^4,$$

where C^1 only conatains terms at least quadratic in y, C^2 only terms at least of degree 1 in y, and $C^4 \in \mathcal{A}_{2m+5}$. Since C^1 and C^2 contain no terms independent of y, they may contribute to the symbol of $\sigma((U_{(23)} \diamond U_{(12)}) \diamond \hat{X} \diamond (U_{(23)} \diamond U_{(12)})^{-1}$ only through higher order terms of the Moyal product. Hence, the whole contribution of C to the symbol is of order $\hbar^{m+2}$.

On the other hand, we see from (4) and $(\Delta\gamma)_{(13)} = (\Delta\gamma)_{(12)} + (\Delta\gamma)_{(23)}$ that $A_{(13)} = A_{(12)} + A_{(13)} + \tilde{C}$, where $\tilde{C} \in \mathcal{A}_{2m+4}$ as well. A close inspection of the possible term in $\tilde{C}$ shows again that it contributes to the symbol of $U_{(13)} \diamond \hat{X} \diamond (U_{(13)})^{-1}$ only at order $\hbar^{m+2}$. Thus, the difference of the two symbols is of order $\hbar^{m+2}$ Q.E.D.

Let $\tilde{\nabla}$ be an arbitrary (possibly $\hbar$-dependent) connection on $V[[\hbar]]$, and π_α a set of projection valued sections in $E[[\hbar]]$ with $\pi_\alpha \pi_\beta = \delta_{\alpha\beta}\pi_\alpha$, $\sum_\alpha \pi_\alpha = \mathrm{id}$. Define $\nabla = \sum_\alpha \pi_\alpha \circ \tilde{\nabla} \circ \pi_\alpha$ as a "Berry type connection". Then $\nabla \pi_\alpha = 0$, and we have the following lemma:

Lemma 3 *With the notations above, and a fixed symplectic connection ∂_s, let $*$ denote the Fedosov star product corresponding to ∇. Then, π_α are "quantum projection", i.e., $\pi_\alpha * \pi_\beta = \delta_{\alpha\beta}\pi_\alpha$.*

Proof: We will show: $\pi_\alpha * \pi_\beta = \pi_\alpha \cdot \pi_\beta$. We first note that, since $\nabla\pi_\alpha = 0\ \forall\alpha$, it follows from (1) that $[r, \pi_\alpha] = 0\ \forall\alpha$ (Since π_α does not depend on y, there is no difference between $\diamond$-commutator and ordinary matrix commutator.) Then, from (2): $\mathcal{Q}(\pi_\alpha) = \pi_\alpha$ for all α. But then we have: $\pi_\alpha * \pi_\beta = \pi_\alpha \cdot \pi_\beta = \delta_{\alpha\beta}\pi_\alpha$. Q.E.D.

3 Berry connections and "block diagonalization"

After the technical preliminaries of the last section, we are now in the position to address the actual problem of this paper.

We consider a Hamiltonian which is a section in the bundle $E[[\hbar]]$:

$$H = H_0 + \hbar H_1 + \dots$$

We assume that the eigenvalues $\lambda_\alpha(x)$ of $H_0(x)$ $(\alpha = 1, \dots r)$, have constant multiplicities m_α throughout phase space. We denote by $\pi_\alpha^{(0)}(x)$ the projections of V_x onto the i-th eigenspace of $H_0(x)$. Under the regularity assumptions above, these eigenspaces form smooth vector bundles over M.

We assume that we are given a hermitian connection on V and a symplectic connection on M, which together define a star product; in many applications there is a distinguished choice of connections and quantization. For example, in the case of the Born-Oppenheimer approximation, one may start with a symplectic manifold which is just the nuclear phase space $\mathbb{R}^{2N}$ where N is three times the number of nuclei in the molecule. In this case, there is a distinguished quantization prescription, namely Weyl ordering, which corresponds to the choice of the trivial connection on the trivial bundle V.

Hence, we assume that we are given a definite quantization. As we allow the symbols of the observables to depend on $\hbar$, one may alternatively interpret this as the choice of a definite symbol calculus.

Nevertheless, we still have the freedom of changing the connection defining our star product without changing the physics, if we apply the corresponding isomorphism of the resulting algebras at the same time, i.e., we have to correct the symbol H by applying the isomorphism ϕ introduced above. We can use this freedom to reduce the problem to a simpler one, which is closer to the scalar case. That this is possible indeed is the content of the next theorem:

Theorem 4 *There exists a formally orthogonal decomposition* $V[[\hbar]] = \oplus_{\alpha=1}^{r} V_\alpha$, $\dim(V_\alpha) = m_\alpha$ *with corresponding quantum projections* $\pi_\alpha^{(\infty)}$ *(i.e.,* $\pi_\alpha^{(\infty)} *_\infty \pi_\beta^{(\infty)} = \delta_{\alpha\beta}\pi_\alpha^{(\infty)}$*), and a compatible connection* $\nabla^{(\infty)}$ *(i.e.* $\nabla^{(\infty)}\pi_\alpha^{(\infty)} = 0\ \forall\alpha$*) such that the corrected symbol* H_{corr} *preserves the decomposition:* $[H_{corr}, \pi_\alpha^{(\infty)}] = 0$ *for* $\alpha = 1, \ldots, r$*. (Here,* $[,]$ *denotes the* $*_\infty$ *commutator).*

Proof: We show the theorem by induction on the order in $\hbar$.

For the connections $\nabla^{(k)}$ to be constructed below we denote by ϕ_k the isomorphism of the algebras $\Gamma(E[[\hbar]])$ with star products $*, *_k$ constructed from ∇ and $\nabla^{(k)}$, respectively: $\phi_k(X * Y) = \phi_k(X) *_k \phi_k(Y)$.

Let $\pi_\alpha^{(1)}(x) \stackrel{\text{def}}{=} \pi_\alpha^{(0)}(x)$ denote the projection onto the i-th eigenspace of $H_0(x)$ (i.e., of the zeroth order term of the original Hamiltonian H), and define $\nabla^{(1)}$ as the Berry-type connection:

$$\nabla^{(1)}\psi \stackrel{\text{def}}{=} \sum_\alpha \pi_\alpha^{(1)} \nabla(\pi_\alpha^{(1)}\psi) \quad .$$

The difference between the corrected Hamiltonian $H^{(1)} = \phi_1(H)$, which is obtained from H by applying the isomorphism corresponding to the change of the connection from ∇ to $\nabla^{(1)}$ is of order $O(\hbar)$ by Lemma 1. Hence, $\nabla^{(1)}\pi_\alpha^{(1)} \equiv 0$ by construction, and $[H^{(1)}, \pi_\alpha^{(1)}] = O(\hbar)$ for all α.

Now assume that we have found (formally orthogonal) projections $\pi_\alpha^{(k)}$ with $\pi_\alpha^{(k)} = \pi_\alpha^{(0)} + O(\hbar)$ with corresponding Berry-type connection

$$\nabla^{(k)}\psi \stackrel{\text{def}}{=} \sum_\alpha \pi_\alpha^{(k)} \nabla(\pi_\alpha^{(k)}\psi)$$

such that the corrected Hamiltonian $H^{(k)} = \phi_k(H)$, satisfies $[H^{(k)}, \pi_\alpha^{(k)}] = O(\hbar^k)$. We will construct new orthogonal projections $\pi_\alpha^{(k+1)}$ satifying the requirement:

$$[H^{(k)}, \pi_\alpha^{(k+1)}] = O(\hbar^{k+1}) \ \ \forall\alpha \tag{6}$$

To this end, we make the ansatz:

$$\pi_\alpha^{(k+1)} = \exp(i\hbar^k A)\pi_\alpha^{(k)} \exp(-i\hbar^k A) \tag{7}$$

for a fixed A independent of α. If we can find such an A, equation (7) automatically defines new formally orthogonal projections (i.e. $\pi_\alpha^{(k+1)} *_{k+1} \pi_\beta^{(k+1)} = \pi_\alpha^{(k+1)}\pi_\beta^{(k+1)} =$

$\delta_{\alpha\beta}\pi_\alpha^{(k+1)}$, according to lemma 3.) With this ansatz $\pi_\alpha^{(k+1)}$ is given up to order $O(\hbar^{k+1})$ by

$$\pi_\alpha^{(k+1)} = \pi_\alpha^{(k)} + i\hbar^k[A, \pi_\alpha^{(k)}] + O(\hbar^{k+1})$$

Hence, equation (6) yields up to order $O(\hbar^{k+1})$ the condition:

$$[H^{(k)}, \pi_\alpha^{(k)}] + i\hbar^k[H_0, [A, \pi_\alpha^{(0)}]] = O(\hbar^{k+1}) \ \ \forall\alpha$$

As the $\pi_\alpha^{(k)}$ are projections, we may write:

$$H^{(k)} = \sum_\alpha \pi_\alpha^{(k)} H^{(k)} \pi_\alpha^{(k)} + \hbar^k W$$

where the first term on the right hand side commutes with $\pi_\alpha^{(k)}$ and

$$\hbar^k W = \sum_{\beta\neq\gamma} \pi_\beta^{(k)} H^{(k)} \pi_\gamma^{(k)} = \sum_{\beta\neq\gamma} \pi_\beta^{(k)} ([H^{(k)}, \pi_\gamma^{(k)}] \pi_\gamma^{(k)}.$$

As the commutator on the right hand side is of order $O(\hbar^k)$ the left hand side is of the same order. Hence, we have to solve:

$$\hbar^k[W, \pi_\alpha^{(0)}] + i\hbar^k[H_0, [A, \pi_\alpha^{(0)}]] = O(\hbar^{k+1}) \ \ \forall\alpha$$

Note that in this equation only the projections $\pi_\alpha^{(0)} \quad (\alpha = 1, \ldots, r)$ appear. A solution to this equation is given by:

$$A = i \sum_{\alpha\neq\beta} \frac{\pi_\alpha^{(k)} W \pi_\beta^{(k)}}{\lambda_\alpha - \lambda_\beta},$$

as may be easily verified using $\pi_\alpha^k W \pi_\alpha^k = 0$ for all α by construction of W.

Using the new projections we may define a new Berry-type connection $\nabla^{(k+1)}$ which preserves the decomposition defined by the projections even to arbitrary order in $\hbar$. As the difference of the projections is of order $O(\hbar^k)$, the difference of the connections $\nabla^{(k)}$ and $\nabla^{(k+1)}$ is of the same order, and hence, by Lemmas 1 2, the corrected symbol $H^{(k+1)} = \phi_{k+1}(H)$ differs from $H^{(k)}$ only at order $O(\hbar^{k+1})$ Thus, by (6), $H^{(k+1)}$ is compatible with the decomposition up to $O(\hbar^{k+1})$: $[H^{(k+1)}, \pi_\alpha^{(k+1)}] = O(\hbar^{k+1})$

As $\nabla^{(k)}$ and $\nabla^{(k+1)}$ differ only at order $O(\hbar^k)$, the connections $\nabla^{(k)}$ have a well defined limit ∇^∞, which by induction fulfills the assertions of the theorem. Q.E.D.

The importance of theorem 4 lies in the following two corollaries:

Corollary 5 *Let $X, Y \in \Gamma E[[\hbar]]$ such that $[X, \pi_\alpha^{(\infty)}] = [Y, \pi_\alpha^{(\infty)}] = 0$ for all α. Let $*_\infty$ denote the star product constructed from $\nabla^{(\infty)}$ by Fedosov's construction. Then $[X *_\infty Y, \pi_\alpha^{(\infty)}] = 0$ for all α.*

Proof: As $\nabla^{(\infty)}\pi_\alpha^{(\infty)} = 0$, the curvature of $\nabla^{(\infty)}$ commutes with $\pi_\alpha^{(\infty)}$. As δ^{-1} only acts on the second factor of $\mathcal{A} = \Gamma(E[[\hbar]] \otimes W)$ and the Moyal product $\diamond$ only involves derivatives with respect to the fibre coordinates y, we may conclude from (1) by induction on the total degree that r commutes with $\pi_\alpha^{(\infty)}$. (Observe that we may write the term $r^2 = r \diamond r$ as $1/2[r,r]_\diamond$).

Now, the covariant constant continuation $\hat{X} = \mathcal{Q}^{(\infty)}(X)$ of X is given by [8]:

$$\hat{X} = X + \delta^{-1}\left(\partial\hat{X} + \left[\frac{i}{\hbar}r, \hat{X}\right]_\diamond\right) \tag{8}$$

and we may again conclude inductively: $[\hat{X}, \pi_\alpha^{(\infty)}] = 0$, and similarly for $\hat{Y}$.

Using again the fact that the Moyal product $\diamond$ on $\mathcal{A}$ only involves derivatives with respect to y, it follows that $\hat{X} \diamond \hat{Y}$ commutes with $\pi_\alpha^{(\infty)}$ for all α. Hence, by taking the symbol, i.e., by setting $y = 0$, we get the assertion of the corollary. Q.E.D.

Corollary 6 *Denote by ϕ_∞ the isomorphism of the algebras $\Gamma(E[[\hbar]])$ with products $*$ and $*_\infty$. Let*

$$\mathcal{O} \stackrel{\text{def}}{=} \{\phi_\infty^{-1}(\tilde{X}) |\ \tilde{X} \in \Gamma(E[[\hbar]]),\ [\tilde{X}, \pi_\alpha^{(\infty)}] = 0\ \forall\alpha\}.$$

Then, $\mathcal{O}$ is a subalgebra of $\Gamma(E[[\hbar]])$ for which the Heisenberg time evolution

$$\dot{X} = \frac{1}{i\hbar}[H, X]_*$$

is a well defined differential equation.

Proof: $\mathcal{O}$ is a subalgebra of $\Gamma(E[[\hbar]])$ by the preceding corollary. We only have to show that $[H, X]_* = O(\hbar)$, since then there will be no negative powers of $\hbar$ in the Heisenberg time evolution.

Denoting again $\phi_\infty(H)$ by H_{corr}, we know that H_{corr} is of the form $\sum_\alpha \lambda_\alpha \pi_\alpha^{(\infty)} + O(\hbar)$.

Now, by (1), r is of the form $r = 1 \otimes \hat{r} + O(\hbar)$ for a scalar one form $\hat{r}$. From this one may conclude that the covariantly constant continuation $\mathcal{Q}^{(\infty)}(H_{corr})$ of H_{corr} is of the form $\sum_\alpha \rho_\alpha \pi_\alpha^{(\infty)} + O(\hbar)$ for some scalar ρ_α. Thus, since $\tilde{X}$ commutes with $\pi_\alpha^{(\infty)}$, we may conclude that the classical matrix commutator does not contribute to $[H_{corr}, \tilde{X}]_{*_\infty}$ at zeroth order in $\hbar$. Hence, the commutator is of order $\hbar$. Applying ϕ_∞^{-1}, the corollary follows. Q.E.D.

4 Correction at order $\hbar$

In the previous section we have achieved a complete reduction of the multicomponent WKB problem to a set of different polarizations. In this section, we will explicitly compute the corrections to the symbol of the Hamiltonian at order $\hbar$. Thus, this

section will generalize the results of [15], and give a completely geometric derivation of the results derived there for trivial bundles only. We achieve this by first using the Berry type connection as in the prove of theorem 4 in the previous section. However, the connection is not uniquely defined by the compatibility conditions: Hence, in the second subsection, we will investigate the dependence of the structure of this phase on the choice of a compatible connection (in the sense of theorem 4). It will turn out that it is unique up to a Berry type phase, and that the Berry type connection considered so far is geometrically distinguished among all compatible connection.

4.1 Berry type connection

To compute the correction of the symbol H at order $\hbar$, we only have to carry out the first two steps of the iterative procedure in the proof of the previous theorem. Actually, it is not necessary to compute $H^{(2)}$, but it is sufficient to compute the "block diagonal" part of $H^{(1)}$ since

$$\begin{aligned} H_{corr} &= H^{(2)} + O(\hbar^2) = \sum_\alpha \pi_\alpha^{(2)} H^{(1)} \pi_\alpha^{(2)} + O(\hbar^2) \\ &= \sum_\alpha \exp(i\hbar A)\pi_\alpha^{(1)} \exp(-i\hbar A) H^{(1)} \exp(i\hbar A)\pi_\alpha^{(1)} \exp(-i\hbar A) \\ &= \sum_\alpha \exp(i\hbar A)\pi_\alpha^{(1)} (H^{(1)} + i\hbar[H^{(1)}, A])\pi_\alpha^{(1)} \exp(-i\hbar A) + O(\hbar^2) \\ &= \sum_\alpha \exp(i\hbar A)\pi_\alpha^{(0)} H^{(1)} \pi_\alpha^{(0)} \exp(-i\hbar A) + O(\hbar^2) \end{aligned}$$

with A as defined in the proof of Theorem 4, and $\pi_\alpha^{(1)} = \pi_\alpha^{(0)}$.

Here, we used the fact that zeroth degree part $H_0^{(1)}$ of $H^{(1)}$ is just $H_0^{(0)}$, and that $\pi^{(0)}$ is the projection onto the eigenspaces of $H_0^{(0)}$. Hence, in order to determine the correction of the symbol at order $\hbar$ up to a unitary rotation, we only have to compute $\pi_\alpha^{(0)} H^{(1)} \pi_\alpha^{(0)}$ for all α.

Defining $\gamma_l \stackrel{\text{def}}{=} \sum_\alpha \pi_\alpha^{(0)} (\nabla_l \pi_\alpha^{(0)})$ we get by formulas (3), (4):

$$\begin{aligned} \pi_\alpha^{(0)} H^{(1)} \pi_\alpha^{(0)} &= \pi_\alpha^{(0)} \Big(H^{(0)} + \sigma([\gamma_l y^l, \nabla_\alpha H_0^{(0)} y^i]_\diamond) \\ &\quad + \frac{1}{2}\sigma([\gamma_l y^l, [\gamma_m y^m, H_0^{(0)}]_{\mathrm{cl}}]_\diamond \Big) \pi_\alpha^{(0)} + O(\hbar^2) \\ &= \pi_\alpha^{(0)} H^{(0)} \pi_\alpha^{(0)} + \pi_\alpha^{(0)} \left(\omega^{il} \frac{i\hbar}{2} \left(\gamma_i \nabla_l H_0^{(0)} - \nabla_i H_0^{(0)} \gamma_l \right) \right) \pi_\alpha^{(0)} \\ &\quad + \pi_\alpha^{(0)} \frac{i\hbar}{4} \omega^{il} \left(\gamma_i [\gamma_l, H_0^{(0)}]_{\mathrm{cl}} - [\gamma_i, H_0^{(0)}]_{\mathrm{cl}} \gamma_l \right) \pi_\alpha^{(0)} + O(\hbar^2) \end{aligned} \tag{9}$$

Here, $[\cdot,\cdot]_{\mathrm{cl}}$ denotes the usual matrix commutator, and $[\cdot,\cdot]_\diamond$ the Moyal product commutator.

In the computation, the following relations (following trivially from the projection property) prove to be useful:

$$\pi^{(0)}_\alpha(\nabla\pi^{(0)}_\beta)\pi^{(0)}_\alpha = 0 \quad \forall\alpha,\beta$$

$$\pi^{(0)}_\alpha(\nabla\pi^{(0)}_\beta)\pi^{(0)}_\beta = \pi^{(0)}_\alpha(\nabla\pi^{(0)}_\beta), \quad \pi^{(0)}_\beta(\nabla\pi^{(0)}_\beta)\pi^{(0)}_\alpha(\nabla\pi^{(0)}_\beta)\pi^{(0)}_\alpha \quad \forall\alpha\neq\beta$$

Using $H^{(0)}_0(x) = \sum_\alpha \lambda_\alpha(x)\pi^{(0)}_\alpha(x)$, we get for the second term on the right hand side of the last equation in (9):

$$\begin{aligned}
&\tfrac{i\hbar}{2}\omega^{il}\Big(\sum_\beta \pi^{(0)}_\alpha(\nabla_i\pi^{(0)}_\alpha)\nabla_l(\lambda_\beta\pi^{(0)}_\beta)\pi^{(0)}_\alpha - \sum_{\beta,\gamma}\pi^{(0)}_\alpha\nabla_i(\lambda_\beta\pi^{(0)}_\beta)\pi^{(0)}_\gamma(\nabla_l\pi^{(0)}_\gamma)\pi^{(0)}_\alpha\Big)\\
&= \tfrac{i\hbar}{2}\omega^{il}\Big(\lambda_\alpha\pi^{(0)}_\alpha(\nabla_i\pi^{(0)}_\alpha)(\nabla_l\pi^{(0)}_\alpha) - \sum_\beta \lambda_\beta\pi^{(0)}_\alpha(\nabla_i\pi^{(0)}_\alpha)\pi^{(0)}_\beta(\nabla_l\pi^{(0)}_\alpha)\\
&\qquad - \sum_\beta \lambda_\beta\pi^{(0)}_\alpha(\nabla_i\pi^{(0)}_\beta)\pi^{(0)}_\alpha(\nabla_l\pi^{(0)}_\alpha) + \sum_{\beta,\gamma}\lambda_\beta\pi^{(0)}_\alpha\nabla_i(\pi^{(0)}_\beta)\pi^{(0)}_\gamma(\nabla_l\pi^{(0)}_\alpha)\Big)\\
&= i\hbar\omega^{il}\sum_\beta \lambda_\beta\pi^{(0)}_\alpha(\nabla_i\pi^{(0)}_\beta)(\nabla_l\pi^{(0)}_\alpha)
\end{aligned}$$

For the last term in (9) we get:

$$\begin{aligned}
&\tfrac{i\hbar}{4}\omega^{il}\Big(\textstyle\sum_{\beta,\gamma}\pi^{(0)}_\alpha(\nabla_i\pi^{(0)}_\alpha)[\pi^{(0)}_\beta\nabla_l\pi^{(0)}_\beta,\lambda_\gamma\pi^{(0)}_\gamma]_{\rm cl}\pi^{(0)}_\alpha\\
&\qquad - \sum_{\beta,\gamma,\rho}\pi^{(0)}_\alpha[\pi^{(0)}_\beta(\nabla_i\pi^{(0)}_\beta),\lambda_\gamma\pi^{(0)}_\gamma]_{\rm cl}\pi^{(0)}_\rho(\nabla_l\pi^{(0)}_\rho)\pi^{(0)}_\alpha\Big)\\
&= \tfrac{i\hbar}{4}\omega^{il}\Big(\lambda_\alpha\sum_\beta\pi^{(0)}_\alpha(\nabla_i\pi^{(0)}_\alpha)\pi^{(0)}_\beta(\nabla_l\pi^{(0)}_\beta)\pi^{(0)}_\alpha - \sum_\gamma\lambda_\gamma\pi^{(0)}_\alpha(\nabla_i\pi^{(0)}_\alpha)\pi^{(0)}_\gamma(\nabla_l\pi^{(0)}_\gamma)\pi^{(0)}_\alpha\\
&\qquad - \sum_\gamma\lambda_\gamma\pi^{(0)}_\alpha(\nabla_i\pi^{(0)}_\alpha)\pi^{(0)}_\gamma(\nabla_l\pi^{(0)}_\gamma)\pi^{(0)}_\alpha + \sum_\rho\lambda_\alpha\pi^{(0)}_\alpha(\nabla_i\pi^{(0)}_\alpha)\pi^{(0)}_\rho(\nabla_l\pi^{(0)}_\rho)\pi^{(0)}_\alpha\Big)\\
&= -\tfrac{i\hbar}{2}\omega^{il}\sum_\gamma\lambda_\gamma\pi^{(0)}_\alpha(\nabla_i\pi^{(0)}_\gamma)(\nabla_l\pi^{(0)}_\alpha)
\end{aligned}$$

Thus, we finally get:

$$\begin{aligned}
\pi^{(0)}_\alpha H^{(1)}\pi^{(0)}_\alpha &= \pi^{(0)}_\alpha H^{(0)}\pi^{(0)}_\alpha + \frac{i\hbar}{2}\omega^{il}\sum_\gamma\lambda_\gamma\pi^{(0)}_\alpha(\nabla_i\pi^{(0)}_\gamma)(\nabla_l\pi^{(0)}_\alpha)\\
&= \pi^{(0)}_\alpha H^{(0)}\pi^{(0)}_\alpha + \frac{i\hbar}{2}\omega^{il}\lambda_\alpha\pi^{(0)}_\alpha(\nabla_i\pi^{(0)}_\alpha)(\nabla_l\pi^{(0)}_\alpha)\\
&\quad + \frac{i\hbar}{2}\omega^{il}\sum_{\gamma\neq\alpha}\lambda_\gamma\pi^{(0)}_\alpha(\nabla_i\pi^{(0)}_\gamma)\pi^{(0)}_\gamma(\nabla_l\pi^{(0)}_\alpha)
\end{aligned}$$

In order to give a geometric interpretation of the correction terms we compute the curvature of the Berry connection:

$$F^B\psi = \sum_\alpha \pi^{(0)}_\alpha\circ\nabla\circ\pi^{(0)}_\circ\nabla\pi^{(0)}_\alpha\psi = \sum_\alpha\pi^{(0)}_\alpha\nabla^2\pi^{(0)}_\alpha + \sum_\alpha\pi^{(0)}_\alpha(\nabla\pi^{(0)}_\alpha)(\nabla\pi^{(0)}_\alpha)$$

$$= \sum_\alpha \pi_\alpha^{(0)} F^o \pi_\alpha^{(0)} + \sum \pi_\alpha^{(0)} (\nabla \pi_\alpha^{(0)}) \wedge (\nabla \pi_\alpha^{(0)})$$

where F^o denotes the curvature of the original connection ∇, and the covariant derivatives have to be interpreted as covariant exterior derivatives, acting on forms.

Hence, the coefficient of λ_α of the α-th block in the correction at order $\hbar$ is $\omega^{-1}(\pi_\alpha^{(0)} F^B \pi_\alpha^{(0)} - \pi_\alpha^{(0)} F^0 \pi_\alpha^{(0)})$. Here, ω^{-1} is the Poisson tensor. The curvature of the Berry connection is block diagonal by construction, the effect of the projection operators on both sides is just to pick out the right block, corresponding to α. In particular, if the original connection is flat, the coefficient of λ_α on the α-th block of the correction is exactly the Poisson curvature of the Berry connection, i.e., the contraction of the curvature with the Poisson tensor.

In order to interpret the remaining terms we define a vector bundle analog of the second fundamental form for embedded submanifolds:

For arbitrary $\beta \neq \alpha$ set

$$\begin{array}{rlll} \tilde{S}^{\beta\alpha}: & \Gamma(V_\alpha^{(1)}) & \to \Gamma(V_\beta^{(1)}) \otimes \Gamma(\Lambda^1(M)) \\ & \psi & \mapsto \pi_\beta^{(1)} \circ \nabla \circ \pi_\alpha^{(1)} \psi = \pi_\beta^{(1)} (\nabla \pi_\alpha^{(1)}) \psi \end{array}$$

$\tilde{S}^{\beta\alpha}$ obviously is tensorial for $\beta \neq \alpha$, hence it induces a mapping $S^{\alpha\beta} : V_\alpha^{(1)} \to V_\beta^{(1)} \otimes \Lambda^1(M)$ which is a vector bundle analog of the second fundamental form: It measures the extent to which parallel transport with respect to ∇ tends to rotate a vector from a given eigenspace into the others.

For fixed $\alpha \neq \beta$, we may form $S^{\beta\alpha} \wedge S^{\alpha\beta}$, which is a two-form with values in the endomorphims of V_α, and hence may be contracted with the Poisson tensor to define an endomorphism of V_α, which is just the coefficient of λ_β in the α-th block of the first order correction of H.

4.2 Arbitrary compatible connection

For an arbitrary connection $\tilde{\nabla}$ which is compatible in the sense of Theorem 4 up to some order $\hbar^k$, we first consider the correction at order $\hbar$. By Lemma 2, we may compute the correction at order $\hbar$ by first going over to the Berry connection, and then in a second step to the connection $\tilde{\nabla}$, as the the corrected symbol obtained in this way differs from he one obtained by going over directly from ∇ to $\tilde{\nabla}$ is of order $O(\hbar^2)$.

As both $\nabla^{(1)}$ and $\tilde{\nabla}$ are compatible with the projections $\pi_\alpha^{(0)}$ up to $O(\hbar)$, the difference $\Delta\gamma$ of the respective connection forms commutes with $\pi_\alpha^{(0)}$ and $H^{(0)}$ up to order $O(\hbar)$. Hence, denoting the corrected symbol corresponding to the new connection $\tilde{\nabla}$ by $\tilde{H}$ we get by formulas (3) and (4) :

$$\begin{aligned} \pi_\alpha^{(0)} \tilde{H} \pi_\alpha^{(0)} &= \pi_\alpha^{(0)} \Big(H^{(1)} + \sigma([(\Delta\gamma)_l y^l, \nabla_i^{(1)} H_0^{(0)} y^i]_\diamond) \\ &\quad + \frac{1}{2} \sigma([(\Delta\gamma)_l y^l, [(\Delta\gamma)_m y^m, H_0^{(0)}]_{\mathrm{cl}}]_\diamond \Big) \pi_\alpha^{(0)} + O(\hbar^2) \end{aligned}$$

$$
\begin{aligned}
&= \pi_\alpha^{(0)} H^{(1)} \pi_\alpha^{(0)} + \pi_\alpha^{(0)} \omega^{il} \frac{i\hbar}{2} \left((\Delta\gamma)_i \nabla_l H_0^{(0)} - \nabla_i H_0^{(0)} (\Delta\gamma)_l \right) \pi_\alpha^{(0)} + O(\hbar^2) \\
&= \pi_\alpha^{(0)} H^{(1)} \pi_\alpha^{(0)} + \pi_\alpha^{(0)} \omega^{il} i\hbar \left((\Delta\gamma)_i (\partial_l \lambda_\alpha) \right) \pi_\alpha^{(0)} + O(\hbar^2) \\
&= \pi_\alpha^{(0)} H^{(1)} \pi_\alpha^{(0)} + \pi_\alpha^{(0)} \omega^{il} i\hbar \left((\Delta\gamma)(X_{\lambda_\alpha}) \right) \pi_\alpha^{(0)} + O(\hbar^2)
\end{aligned}
$$

Here, X_{λ_α} denotes the Hamiltonian vector field corresponding to λ_α.

Hence, we see that for an arbitrary connection compatible with $\pi_\alpha^{(0)}$ the lowest order corrections differ just by a Berry phase term. The additional geometric term involving the eigenvalues themselves and not their derivatives are unique and always contain the Poisson curvature and the second fundamental form of the Berry-connection and *not* the Poisson curvature of the chosen connection. Hence, the Berry connection is distinguished among all connections satisfying Theorem 4.

5 Outlook

In the preceding sections, we have achieved a complete block diagonalization of the considered problem: We have found a decomposition of $V[[\hbar]]$ into subspaces, such that the symbol of the Hamiltonian and the connection are compatible with this decomposition. Furthermore, we have found a maximal set of observables which is compatible with this decomposition as well in that sense, that their time evolution does not contain any negative powers of $\hbar$. Hence, for the purposes of WKB approximation, one may treat each block separately.

However, the problem of multicomponent WKB has not been completely reduced to a scalar problem. In this section, we will show that it can still be reduced closer to a purely scalar one, but only at the price of non-canonical choices of a connection. Nevertheless, this further reduction proves to be useful for a discussion of obstructions to a complete reduction to a scalar problem. Furthermore, for this discussion, only parallel transport along the Hamiltonian vector field will play a role, which does not depend on the choices made in the connection:

We have seen in the last section that the choice of a different connection leads at order $\hbar$ to the addition of a Berry-phase term $\gamma(X_{\lambda_\alpha})$ to the α-th block of the corrected symbol. We may use the Berry-phase term to simplify the problem by choosing the connection such that this term just compensates the remaining terms at order $\hbar$, so that the Hamiltonian is reduced to a set of scalar Hamiltonians up to order $O(\hbar^2)$ on the αth block. This is always possible as long as the eigenvalue functions have no critical points, where their hamiltonian vector fields vanish. In practice this means that one has to cut out those points. However, this is not a real problem if one has applications to WKB in mind, as the Lagrangian submanifolds relevant to the WKB approximation lie in level sets of the eigenvalue functions and hence will generically not intersect the critical points. It is possible to iterate the procedure above, which gives the following theorem:

Theorem 7 *Let $\tilde{M}$ be any open submanifold of M not containing critical points of the eigenvalue functions λ_α. Denote the embedding of $\tilde{M}$ by i, and let $\tilde{V}$ be the pull*

back bundle $i^*(V)$, i.e., the subbundle of V obtained by restricting V to $\tilde{M}$. Then, there is an ($\hbar$ dependent) connection $\tilde{\nabla}^\infty$ and a decomposition $\tilde{V}[[\hbar]] = \oplus_{\alpha=1}^m \tilde{V}_\alpha$ fulfilling Theorem 4 such that the corrected Hamiltonian restricted to $\tilde{V}_\alpha$ is scalar, namely the eigenvalue function λ_α of $H^{(0)}$ for each α.

As stated before, the connection defined in this way is far from unique: Only the partial connection for each block, giving covariant derivatives in the direction of the respective Hamiltonian vector field, is uniquely defined by the iteration procedure above. However, we may always find a continuation of this partial connection to a connection on the whole bundle.

The result of Theorems 4 and 7 is optimal in the following sense: We started from a decomposition of V into the bundles of eigenvectors of H_0. However, due to the higher order corrections, the eigenvalues of the quantum mechanical Hamiltonian operator will in general have lower degeneracy than the eigenvalues of the principal symbol H_0. One might hope to find a finer decomposition of the vector bundle $V[[\hbar]]$, so that one ends up with one dimensional subbundles and "formal $U(1)$-connections". However, this is not possible in general, not even at order $O(\hbar^2)$: The connection constructed in the previous theorem has in general a $U(m_1) \times \ldots U(m_r)$ holonomy and cannot be replaced by a connection with a $U(1) \times \ldots \times U(1)$ holonomy without destroying the block-diagonality of the corrected symbol of the Hamiltonian.

To understand this fact better, we first consider the case of a two dimensional phase space as base space. In this special case it is always possible to reduce the problem to one-dimensional subbundles, at least in a tubular neighborhood of any energy level set $\lambda_\alpha^{-1}(E)$ for a non-critical value E:

To show the existence of such a decomposition and a compatible connection we start with a connection $\tilde{\nabla}^\infty$ for which the Hamiltonian is scalar on each block, as in theorem 7. As the connection to be defined will respect the block structure, we may restrict ourselves to one block α and only need to consider the corresponding eigenvalue function λ_α.

If $\lambda_\alpha^{-1}(E)$ is diffeomorphic to $\mathbb{R}$, we may choose a transversal manifold S at some point $p \in \lambda_\alpha^{-1}(E)$. Choosing an arbitrary decomposition into one-dimensional subbundles on S, we may define a decomposition on a whole tubular neighborhood of $\lambda_\alpha^{-1}(E)$ by parallel transport along the Hamiltonian flow of λ_α. Denoting by $\tilde{\pi}_k$ the corresponding one-dimensional projections, we define a new connection $\hat{\nabla}$ as $\sum_k \pi_k \circ \tilde{\nabla}^\infty \circ \pi_k$. Since we have a set of trivializing sections covariantly constant along the Hamiltonian flow both for $\tilde{\nabla}^\infty$ and for $\hat{\nabla}$, it follows:

$$\hat{\nabla}_{X_{\lambda_\alpha}} u = \tilde{\nabla}^\infty_{X_{\lambda_\alpha}} u$$

for any section u in the the α-th block, and hence the corrected symbol is not modified at order $\hbar$ by going over to the new connection. Hence, the Hamiltonian is still scalar (at least up to order $O(\hbar^2)$, and we have found the connection and decomposition we are looking for up to the same order. This procedure can be iterated again, and we can thus reduce the problem to a purely scalar one.

If $\lambda_\alpha^{-1}(E)$ is diffeomorphic to S^1, then the situation is a bit more involved: Due to the periodicity of the flow, we cannot simply define a decomposition into subbundles on a complete tubular neighborhood of the level set by parallel transport of an arbitrary decomposition on a transversal submanifold S. Instead, defining $U(p)$ as the holonomy for $\tilde{\nabla}^\infty$ along one period of the Hamiltonian flow line starting at the point $p \in S$, we choose the complex eigenspaces of $U(p)$ (which always exist as U is unitary) on S and parallel transport these along the Hamiltonian flow of λ_α. (If the eigenspaces of U are not one-dimensional then we have to choose one dimensional subspaces in a smooth way along S.) We may define $\hat{\nabla}$ as before and get a connection with the desired properties.

We note that we can even modify the connection further by adding a $u(1) \times u(1)$-valued one-form to the connection form such that the holonomy along the Hamiltonian flow vanishes and the symbol of the Hamiltonian is modified without destroying diagonality: The corresponding phase is moved in this way from the connection to the symbol.

These observations explain the special role of two-dimensional phase spaces for multicomponent WKB approximation. Now, an analogous construction obviously does not work generally if the underlying phase space is more than two dimensional: Even if the Hamiltonian system defined by λ_α is integrable, the flow will generically be only quasiperiodic. This does not only imply that the above construction does not work, but even that such a decomposition into one dimensional subbundles with a compatible connection and scalar symbols does not exist:

Namely, assume such a decomposition would exist. Let γ denote the integral curve of X_{λ_α} through a fixed point p. Then (pulling back the respective bundles with the inclusion map $i : \gamma \to M$) we first claim that the decomposition of $i^*V[[\hbar]]$ into one-dimensional subbundles is uniquely determined by the decomposition at the point p and the requirement that the corrected symbol is diagonal with respect to the decomposition. To see this, we first note that given any such decomposition with compatible connection, it is determined by the decomposition at P through parallel transport. Hence, if there are several such decompositions, they must correspond to different connections.

However, we may modify any such connection without changing the decomposition by adding a $u(1) \times \ldots \times u(1)$ valued one-form to the connection form. By a proper choice, we may achieve that the corrected symbol on the α-th block is simply λ_α. Now assume that we are given two different decompositions with corresponding (properly modified) connections which coincide at the point p. Then, as the corrected symbols simply is λ_α in both cases, the difference of the connection forms of the two connections (modified as above) must vanish on X_{λ_α}, hence parallel transport along γ coincides for both connections. As the decomposition has to be invariant under parallel transport, the two decomposition must coincide over γ.

Hence, there is at most one such decomposition, and it determined by parallel transport with the connection in theorem 7. Now, due to the quasi-periodicity, the curve γ comes arbitrarily close to p for certain arbitrarily large times T_i. However, there will generically be no one-dimensional subspace W_p in the fiber V_p over p which,

when parallel transported along γ, will be in a suitable sense close to W_p for all the times T_i. Hence, there cannot exist a continous decomposition into one-dimensional subspaces with the desired properties which is defined in a whole neighborhood of γ.

The difference to the situation in perturbation theory comes from the Berry-phase term. Hence, if one tries to completely diagonalize the corrected symbol, one has to solve a differential equation along the flow of λ_α, and not just simply to diagonalize a matrix. Thus, although it is always possible to completely diagonalize the symbol locally, this is not possible in general globally.

References

[1] Bates, S.M., and Weinstein, A., Lectures on the Geometry of Quantization, *Berkeley Mathematics Lecture Notes*

[2] F. Bayen, M. Flato, C. Fronsdal, A. Lichnerowicz, D. Sternheimer: Deformation Theory and Quantization. *Annals of Physics* **111** (1978), part I: 61-110, part II: 111-151.

[3] Berry, M.V., Quantal phase factors accompanying adiabatic changes, *Proc. R. Soc. London A* **392** (1984), 45-57.

[4] Cordes, H.O., A pseudo-algebra of observables for the Dirac equation, *Manuscripta Math.* **45** (1983), 77-105.

[5] Dencker, N., On the propagation of polarization sets for systems of real principal type, *J. Funct. Anal.* **46** (1982), 351-372.

[6] M. DeWilde, P.B.A. Lecomte: Existence of star-products and of formal deformations of the Poisson Lie Algebra of arbitrary symplectic manifolds. *Lett. Math. Phys.* **7** (1983), 487-496.

[7] Duistermaat, J. J., Fourier Integral Operators,*Courant Institute*, NYU, New York, 1973.

[8] Fedosov, B., A Simple Geometrical Construction of Deformation Quantization, J. of Diff. Geom. **40** (1994), 213-238.

[9] Fedosov, B., Reduction and eigenstates in deformation quantization, In *Pseudo-Differential Calculus and Mathematical Physics, Advances in Prtial Differential Equations*, Akademie Verlag, Berlin 1994, 227-297

[10] Guillemin, V., and Sternberg, S., Geometric Asymptotics, *Math. Surveys* **14**, Amer. Math. Soc., Providence, 1977.

[11] Hörmander, L., Fourier Integral Operators I., *Acta Math.* **127** (1971) 79-183.

[12] Karasev, M.V., New global asymptotics and anomalies for the problem of quantization of the adiabatic invariant, *Funct. Anal. Appl.* **24** (1990), 104-114.

[13] Karasev, M.V., and Maslov, V.P., Operators with general commutation relations and their applications. I. Unitary-nonlinear operator equations, *J. Sov. Math.* **15** (1981), 273-368.

[14] Klein, M, Martinez, A, Wang X.P., On the Born-Oppenheimer Approximation of Wave Operators in Molecular Scattering Theory, *Comm. Math. Phys.* **152** (1993), 73-95

[15] Littlejohn, R.G., and Flynn, W.G., Geometric phases in the asymptotic theory of coupled wave equations, *Phys. Rev.* **A44** (1991), 5239-5256.

[16] Maslov, V.P., and Fedoriuk, M.V., Semi-classical Approximation in Quantum Mechanics, D. Reidel, Dordrecht, 1981.

[17] Emmrich, C., and Weinstein, A., Geometry of the transport equation in multicomponent WKB approximation, *Comm. Math. Phys.* **176** (1996), 701-711

[18] Yabana, K., Horiuchi, H., Adiabatic Viewpoint for the WKB Treatment of Coupled Channel Systems, *Prog. Theor. Phys.* **75** (1986), 592-618